REPORT DOCUMENTATION PAGE

Form Approved
OMB No. 0704-0188

1. REPORT DATE *(DD-MM-YYYY)* 21-07-2011	**2. REPORT TYPE** Briefing Slides	**3. DATES COVERED** *(From - To)*
4. TITLE AND SUBTITLE **Stability of Flame-Shock Coupling in Detonation Waves: 1D Dynamics**		**5a. CONTRACT NUMBER** **5b. GRANT NUMBER** **5c. PROGRAM ELEMENT NUMBER**
6. AUTHOR(S) Lord K. Cole, Jean-Luc Cambier, and Ann R. Karagozian		**5d. PROJECT NUMBER** **5f. WORK UNIT NUMBER** 33SP0853
7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) Air Force Research Laboratory (AFMC) AFRL/RZSS 1 Ara Road Edwards AFB CA 93524-7013		**8. PERFORMING ORGANIZATION REPORT NUMBER** AFRL-RZ-ED-VG-2011-321
9. SPONSORING / MONITORING AGENCY NAME(S) AND ADDRESS(ES) Air Force Research Laboratory (AFMC) AFRL/RZS 5 Pollux Drive Edwards AFB CA 93524-7048		**10. SPONSOR/MONITOR'S ACRONYM(S)** **11. SPONSOR/MONITOR'S NUMBER(S)** AFRL-RZ-ED-VG-2011-321

12. DISTRIBUTION / AVAILABILITY STATEMENT

Approved for public release; distribution unlimited (PA #11332).

13. SUPPLEMENTARY NOTES

For presentation at Academia UC Irvine, 28 July 2011.

14. ABSTRACT

This briefing explores the stability of flame-shock coupling in detonation waves: 1D dynamics.

15. SUBJECT TERMS

16. SECURITY CLASSIFICATION OF:			**17. LIMITATION OF ABSTRACT**	**18. NUMBER OF PAGES**	**19a. NAME OF RESPONSIBLE PERSON**
a. REPORT	**b. ABSTRACT**	**c. THIS PAGE**			Justin W. Koo, Ph.D.
Unclassified	**Unclassified**	**Unclassified**	SAR	27	**19b. TELEPHONE NUMBER** *(include area code)* N/A

Standard Form 298 (Rev. 8-98)
Prescribed by ANSI Std. 239.18

Stability of Flame-Shock Coupling in Detonation Waves: 1D Dynamics

Lord K. Cole[1], Jean-Luc Cambier [2], Ann R. Karagozian[1]

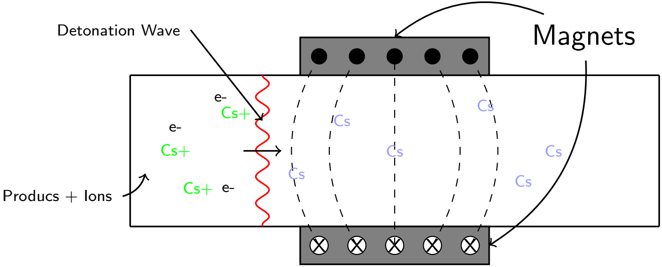
[1]Department of Mechanical and Aerospace Engineering
University of California, Los Angeles

[2]Air Force Research Laboratory, Spacecraft Branch
Edwards AFB, CA 93524

28 July 2011

Motivation

- How will energy extraction/introduction via joule heating($\vec{J} \cdot \vec{E}$) affect the stability of the detonation?
- How will the magnetic Pressure($\vec{J} \times \vec{B}$) evolution affect the Reaction Zone and detonation stability?



Goals of the Present Study

- In order to understand detonation-magnetic field interactions, one must first understand the stability criteria of an unmagnetized, unsupported detonation.
- Explore the nonlinear dynamics involved in detonation stability
  - Induction lengths relation to kinetics & dynamics
- Examine the coupling of large and small length scale physics
  - Correlating different modes of peak pressure behavior to small scale phenomena

Numerical Methodology

Inviscid, one-dimensional Euler equations using multi-step,reversible reaction mechanism:

$$\mathbf{Q}_t + \mathbf{F}(\mathbf{Q})_x = \mathbf{S}(\mathbf{Q}) \tag{1}$$

where the vectors represented by Q, F, and S are, respectively,

$$\mathbf{Q} = \begin{pmatrix} \rho_s \\ \rho u \\ \hat{E} \end{pmatrix}, \mathbf{F} = \begin{pmatrix} \rho_s u \\ \rho u^2 + P \\ (\hat{E} + P)u \end{pmatrix}, \mathbf{S} = \begin{pmatrix} \omega_s \\ 0 \\ \sum_s \omega_s e_{0s} \end{pmatrix} \tag{2}$$

where the total mixture density $\rho = \sum_s \rho_s$, and the total energy $\hat{E}$ may be written

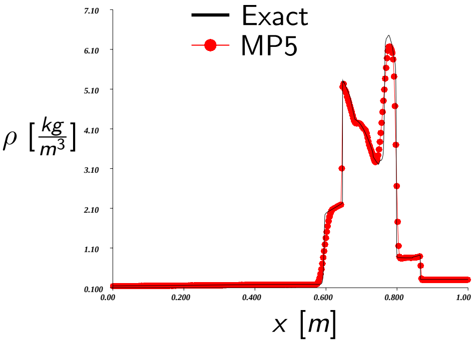
$$\hat{E} = \rho \int c_v(T)dT + \frac{1}{2}\rho u^2 \tag{3}$$

Numerical Schemes

- Monoticity Preserving(MP) Schemes (Suresh & Huynh, 1997)
  - 5^{th} order spatial discretization was used in conjuction with 3^{rd} order TVD-Runge-Kutta time integration
  - Contact Discontinuities well resolved without the use of artificial compression methods
- Advection-Diffusion-Reaction Weighted Essential Non-Oscillatory(ADERWENO) Scheme (Titarev & Toro, 2001)
  - 5^{th} order spatial and 3^{rd} order temporal without Runge-Kutta time integration
  - Utilizes Lax-Wendroff procedure and Taylor series expansion of WENO fluxes for high order in time

Validation Studies

- Euler equation solutions using MP schemes validated for standard problems:
  - Sod's 1D Shock tube problem
  - Lax's 1D problem, shock tube with velocity field
  - Shu-Osher 1D problem, entropy wave-shock interaction
  - 1D Blastwave problem, e.g.,



300 grid points

Ideal MHD Conservation Equations

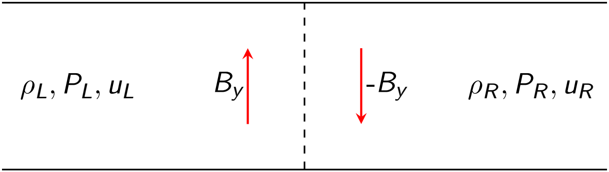
$$\mathbf{Q}_t + \mathbf{F}_x = 0$$

$$\mathbf{Q} = \begin{pmatrix} \rho_s \\ \rho\mathbf{u} \\ \mathbf{B} \\ E \end{pmatrix}, \quad \mathbf{F} = \begin{pmatrix} \rho_s u_n \\ \rho\mathbf{u}u_n + P^*\mathbf{n} - \mathbf{B}B_n \\ u_n\mathbf{B} - \mathbf{u}B_n \\ (E + P^*)\,u_n - B_n\,(\mathbf{u}\cdot\mathbf{B}) \end{pmatrix}$$

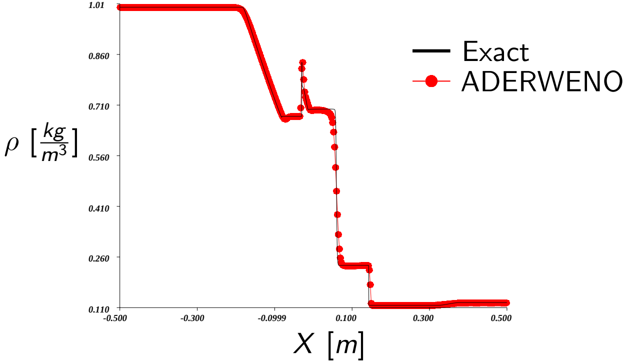
where

$$B_n = B_x n_x + B_y n_y + B_z n_z, \quad P^* = P + \tfrac{1}{2}\|\mathbf{B}\|^2$$

Validated for standard 1D Brio-Wu Problem, analogous to Sod's shock tube:



1D Brio-Wu validation with ADERWENO



Initial Conditions:

$$\{\rho_L, P_L, u_L, B_x, B_y\} = \{1\frac{kg}{m^3}, 10^5\ \text{Pa}, 0\frac{m}{s}, 0.75, 1\}$$

$$\{\rho_R, P_R, u_R, B_x, B_y\} = \{0.125\frac{kg}{m^3}, 10^4\ \text{Pa}, 0\frac{m}{s}, 0.75, -1\}$$

Chemical Kinetics Conservation Equations

Operator-Splitting

$$\frac{d\mathbf{Q}}{dt} = \mathbf{S}$$

where

$$\mathbf{Q} = \begin{pmatrix} \rho_s \\ \rho\mathbf{u} \\ E \end{pmatrix}, \mathbf{S} = \begin{pmatrix} \dot{\omega}_s \\ 0 \\ \sum \dot{\omega}_s e_{0s} \end{pmatrix}$$

$$\dot{\omega}_s = \sum_r \nu_{rs} k_{fr} \prod_j [X_j]^{\nu'_{rj}} - \sum_r \nu_{rs} k_{br} \prod_j [X_j]^{\nu''_{rj}}$$

$$\nu_{rk} = \nu''_{rk} - \nu'_{rk}$$

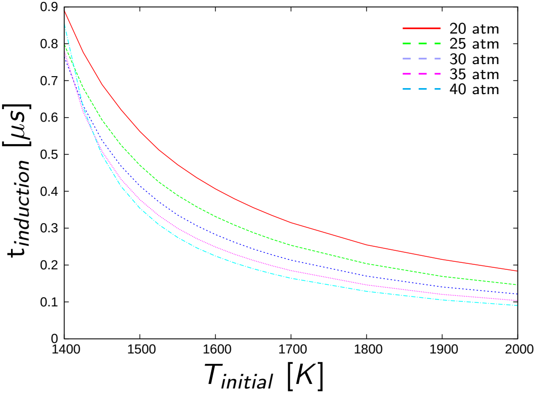
ν''_{rk}: coefficient of k^{th} species in the r^{th} forward reaction
ν'_{rk}: coefficient of k^{th} species in the r^{th} reverse reaction
$[X_s]$: Concentration of s^{th} species
e_{0s}: Internal Energy of formation at $0K$

Kinetics of Hydrogen-Air Mixture:

- The chemistry includes eight reacting species, H_2, O_2, H, O, OH, HO_2, H_2O_2, H_2O, and the non-reacting diluent N_2.
- Thirty eight elementary reactions are used in this mechanism and the backward rates are computed from equilibrium constants.
- Convection and Kinetics were operator split
  - Point Implicit Euler was used to solve for the kinetics

Induction Delay Time

Reduced $H_2 - O_2 - N_2$ Reaction Kinetics (9 species, 38 reactions)

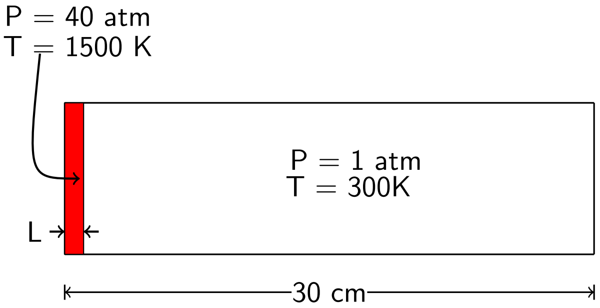


Can be fitted as $t \sim \alpha(P)e^{\frac{\beta(P)}{T}}$

Criterion for Induction: Maximum atomic Hydrogen concentration

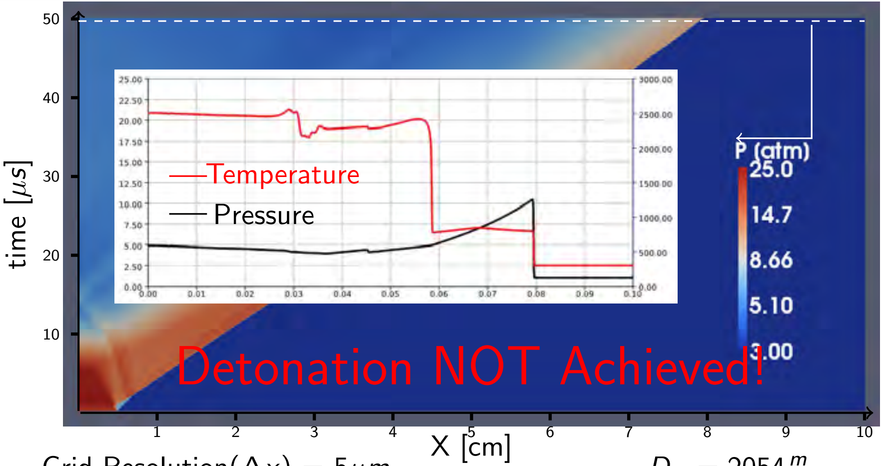
Mixture: Stochiometric $H_2 - O_2 - N_2$

Detonation Test Setup



- Premixed Stoichiometric Mixture of H_2−Air
- Closed Ends
- Spark ignited (L = 0.25 cm in the Present Study)
- $D_{cj} \approx 2054 m/s$

Spark Ignited Detonation – Pressure Contour (MP5)



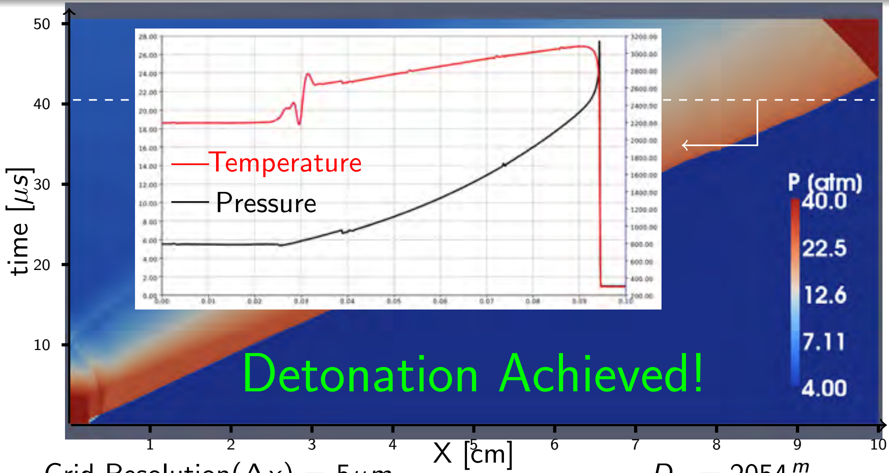
Grid Resolution(Δx) $= 5\mu m$

L $=$ 0.5 cm

$D_{cj} = 2054\frac{m}{s}$

$D = 1500\frac{m}{s}$

Spark Alteration (P_{spark} = 50 atm, L = .25cm), MP5



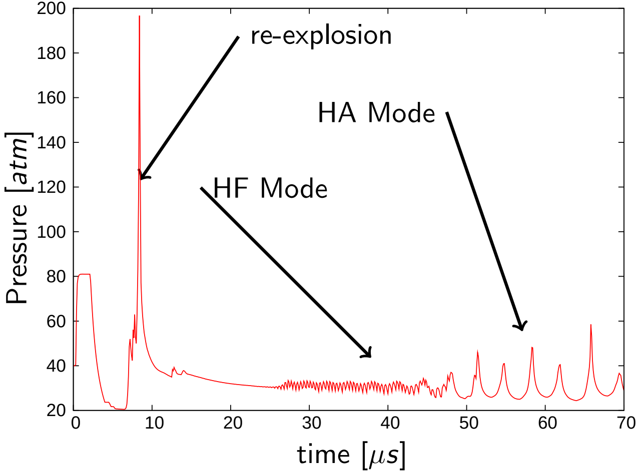
Grid Resolution(Δx) = 5μm
L = 0.25 cm

$D_{cj} = 2054\frac{m}{s}$
$D = 2031\frac{m}{s}$

Typical Peak Pressure vs Time Plot

Grid Resolution: $\Delta x = 2.5\mu m$

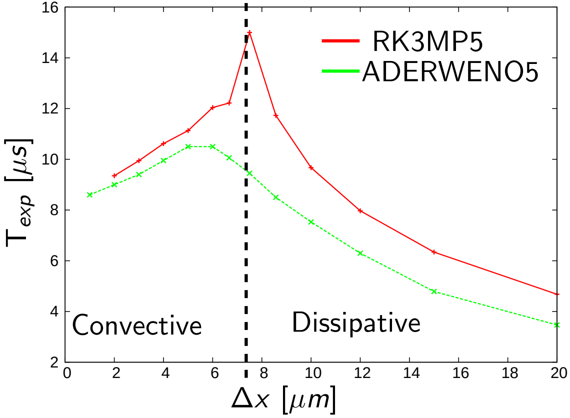
HF- High Frequency, HA- High Amplitude



Time to Re-Explosion

Time of re-explosion(T_{exp}):

- criteria P $>$ 100 atm

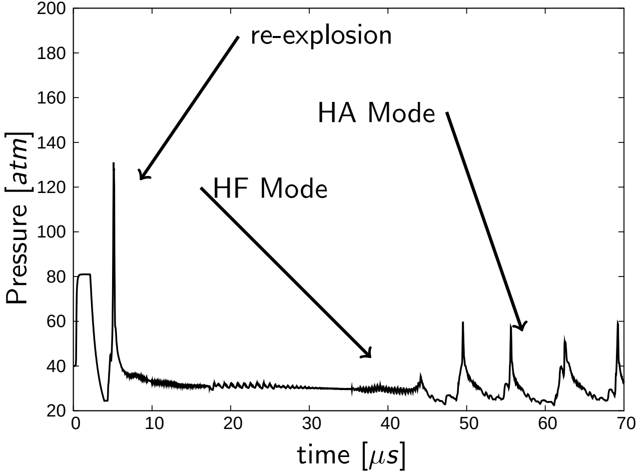


Grid Convergence

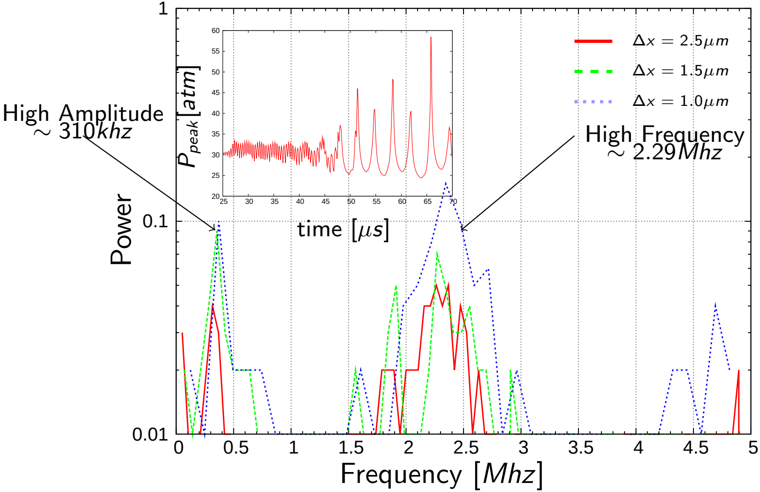
- Peak Pressure vs Time data relates macroscopic phenomena to microscopic phenomena
- Spectral content of the High Frequency and High Amplitude Modes for various grid resolution can be used to determine convergence
- High Frequency modes were inconsistent as the grid resolution increased to $\Delta x \geq 7.5 \mu m$

Typical Peak Pressure vs Time Plot

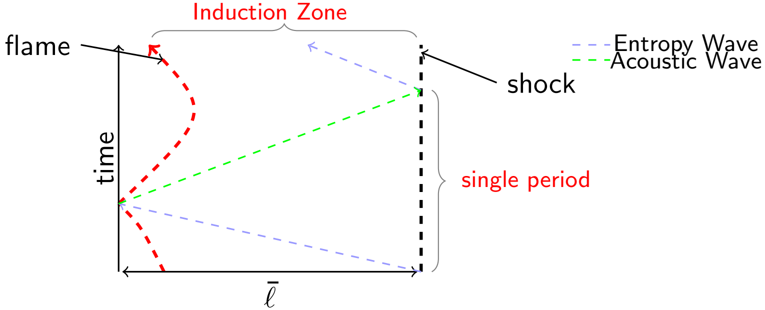
Grid Resolution: $\Delta x = 12.5\mu m$



Spectral Convergence



Simplified Model
Induction Zone Dynamics

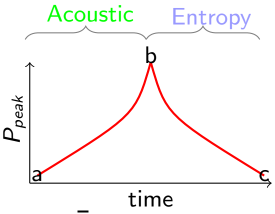


$$\left.\frac{dx}{dt}\right|_{entropy} = u_2(x,t) \tag{4}$$

$$\left.\frac{dx}{dt}\right|_{acoustic} = c(x,t) - u_2(x,t) \tag{5}$$

where $u_2(x,t) = |u(x,t) - D(t)|$ (detonation ref. frame)

Verify Simple Model



$$\mathcal{T} = \frac{\bar{\ell}}{c_a + u_a - \bar{D}_{a\rightarrow b}} + \frac{\ell}{u_b - \bar{D}_{b\rightarrow c}} \tag{6}$$

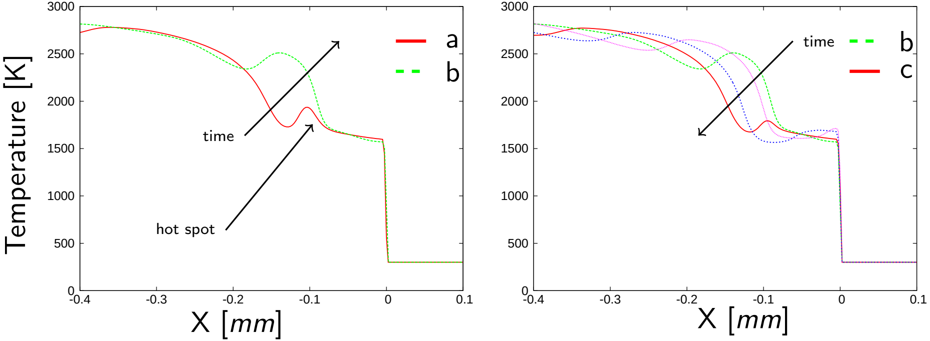
$$f = \mathcal{T}^{-1}, \text{ frequency}$$

Assumptions for zeroth order approximation:

- $\bar{D} = \frac{1}{\mathcal{T}} \int D(t)dt$
- $\gamma \approx 1.28$
- T, P, ρ, u $\rightarrow F(x,t)$, $\quad \frac{\partial F(x,t)}{\partial t} \simeq 0$ & $\frac{\partial F(x,t)}{\partial x} \simeq 0$

Verify Simple Model

High Frequency Mode

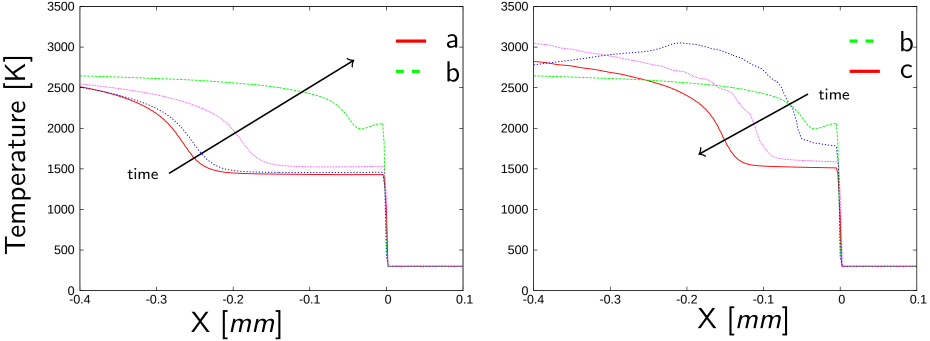


a: $29.1\mu s$ b: $29.3\mu s$ c: $29.5\mu s$

$f \approx 2.08\ Mhz$, In good agreement with spectral analysis ($2.29 \pm 0.4\ Mhz$)

Verify Simple Model

High Amplitude Mode



a: $56.7\mu s$ b: $58.3\mu s$ c: $60.1\mu s$

$f \approx 310\ khz$, In great agreement with spectral analysis ($310 \pm 40\ khz$)

Conclusions

- Same fundamental dynamics for High Frequency and High Amplitude Modes
- The location of the hot spot, whether within the flame or reaction zone, plays a key role in pressure oscillations.
  - ‘hot spot’ inhibits progress of flame toward shock by pre-igniting fluid, thus suppressing the peak amplitude of pressure
- HF Mode: “hotspot” well resolved within induction zone, leading to small fluctuations in Pressure
- HA Mode: fluctuations are within flame, allowing for more energy release (via Swacer effect)

Future Work

- Conduct similar test with a seeded species of low ionization energy and direct initiation (Hydrocarbon fuel)
  - Observe how ionization processes effect the induction region and large scale phenomena
- Apply B-field of varying strength

Backup
MHD Effects

Additional Physics added in MHD

$$\begin{aligned} \vec{F} &= \vec{J} \times \vec{B} && \text{Lorentz Force} \\ Q &= \vec{J} \cdot \vec{E} && \text{Joule Heating} \end{aligned} \tag{7}$$

Questions:

- How will energy extraction/introduction via joule heating effect the stability of the detonation?
- How will the magnetic Pressure evolution effect the Reaction Zone & detonation stability?